Development of a Simulation Force Field for Equilibrium and Transport Property Calculations

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Computer hardware and simulation methodologies have developed to the extent that fluid property simulations are routine in academia. Simulation has developed to a state where it can be used to answer questions that cannot be addressed by conventional experimentation and can provide data that can be used to test and validate theories. A measure of this development is the growing acceptance of simulation in industry. Westmoreland et al.[1] have reported that molecular modeling methods have gained acceptance as practical tools in a variety of industries including pharmaceuticals, agricultural chemicals, commodity and specialty chemicals, fuels, polymers, and personal-care and food products amongst others. Nonetheless, application of simulation methodology in industry is not routine, primarily due to uncertainties in the force fields required for accurate simulation.

During the past five years, there have been notable advances in developing force-field models using phase equilibrium data. It is also fair to say that good progress has been made in the transferability of force fields for equilibrium properties between molecules, but problems remain with the overall transferability of the models for different thermophysical properties. One can generalize that essentially all of the force fields proposed for equilibrium properties tend to substantially underestimate the dense phase viscosity. In this work we have developed a new united atom force field that can be applied to both equilibrium and non-equilibrium property simulations. The non-bonded part of the force field features a softer repulsion and more complex long-range attraction. In this presentation we present results of equilibrium and transport property simulations and compare these results with experimental data and results obtained with other force fields.

1. P. R. Westmoreland, P. A. Kollman, A. M. Chaka, P. T. Cummings, K. Morokuma, M. Neurock, E. M. Stechel, and P. Vashishta Applying Molecular and Materials Modeling: An International Comparative Study. (Kluwer Academic, New York, NY, 2002).